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Computational Insights into Thiosemicarbazone Metal Complexes: Structural Elucidation, Reactivity Patterns, and Biomedical Implications

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INTRODUCTION

- Computational studies of thiosemicarbazone(TSC) metal complexes play a crucial role in elucidating their structural, electronic, and reactivity properties, thus contributing significantly to various scientific fields.
- Thiosemicarbazone ligands are renowned for their versatile coordination behavior and diverse biological activities, making their metal complexes subjects of keen interest in chemistry and related disciplines.
- Computational studies offer a cost-effective and time-efficient approach to explore the structures, properties, and applications of thiosemicarbazone metal complexes[1].

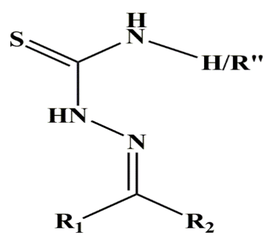


Fig. 1. General structure of TSC ligand

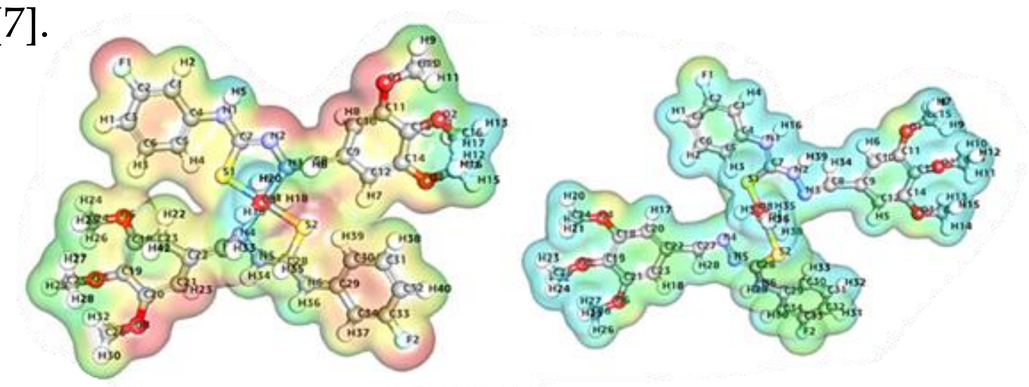
METHODOLOGY

- Geometry optimization and frequency calculations were carried out with Gaussian and GaussView programme by using DFT[2].
- B3LYP Method and 6-311G (d,p)/6-31+G(d,p) basis sets were used.
- Metal ions were characterized by the nonrelativistic effective core potential (ECP) LANL2DZ relativistic pseudopotential.

DFT/Biological Applications of TSC-Metal complexes

❖ Molecular electrostatic potential (MESP) analysis

The blue color denotes the molecule's electronically weak regions and the red color represents the electron-rich regions[7].

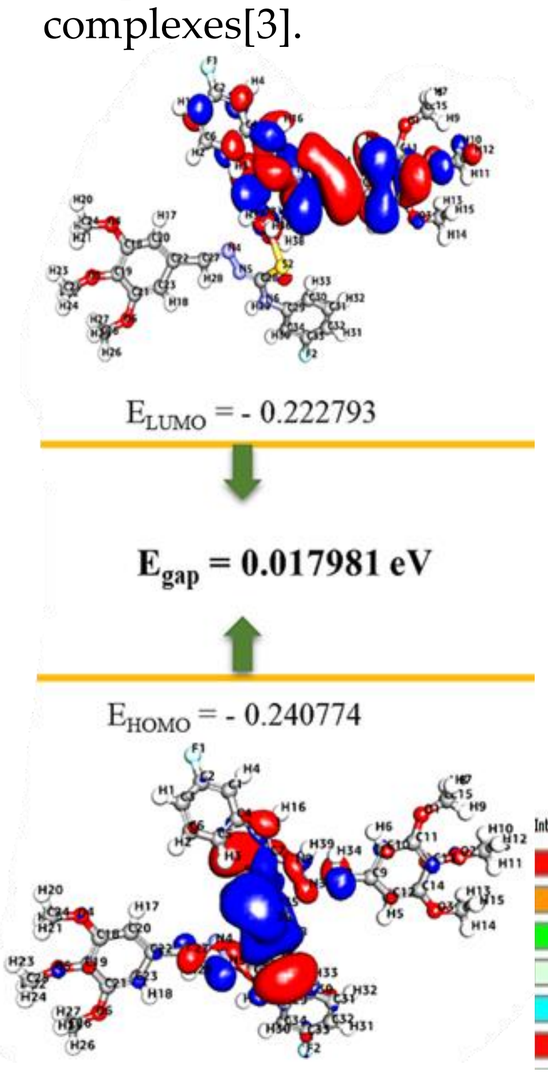


M= Ni, Cu

Fig. 2. Fluoro substituted–TSC Complexes

❖ HOMO-LUMO & Molecular Docking Analysis

- The energy gap (E_g) between HOMO and LUMO (Fig. 3a) is very useful in explaining the properties of a molecule, such as chemical stability and electronic parameters[3].
- Molecular docking (Fig. 3b) study is carried out to analyze the binding energies and binding interactions of the compounds against the active site of amino acids of the protein. It helps in choosing relevant biological targets, such as enzymes or receptors involved in diseases, for thiosemicarbazone complexes[3].



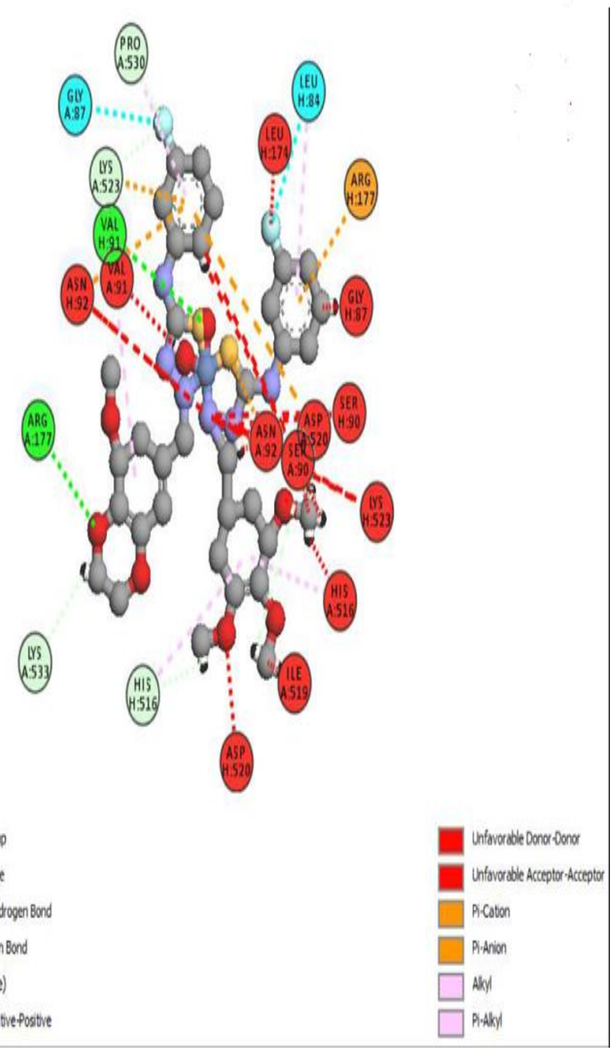


Fig. 3. HOMO-LUMO (a)& Docking(b) plot of Ni-TSC complex

CONCLUSION

Thiosemicarbazone metal complexes exhibit diverse structures and reactivity patterns, with DFT studies crucial for understanding their potential in biomedical applications.

FUTURE WORK / REFERENCES

1. Gupta, et al. 2022, *Results in Chemistry*, 4, 100459.
2. Frisch et al.2016. G16_C01. Gaussian 16, Revision C. 01, Gaussian. *Inc., Wallin*, *248*.
3. Kumar, et al. 2024,*Inorganic Chemistry Communications* 159.
4. Devi, Jai, et al. 2024, *Biometals* 37.1, 247-265.
5. Jan, Faheem, et al. ,2024 *Journal of Molecular Structure*, 138459.